How Simulations Clarify Complex Material Phase Transitions

Kurt Binder, Marcus Müller, and Friederike Schmid

ATOMISTIC SIMULATIONS CAN CLARIFY PHASE TRANSITIONS OF "SIMPLE" SYSTEMS, FORMED FROM ATOMS OF A PURE SUBSTANCE OR FROM SMALL MOLECULES, IN QUANTITATIVE DETAILS. MORE COMPLEX MATERIALS (such as surfactant layers or polymer mixtures) require coarse-grained models, but the predictive capability for specific chemical properties of nature is lost. Nevertheless, studies using such coarse-grained models are very useful because they give insight into the generic features responsible for a particular phase's behavior. Two specific examples illustrate this gained insight, namely the phase diagram of dense, fluid Langmuir monolayers and the unmixing of polymer blends in a thin-layer geometry.

Since Monte Carlo and molecular dynamics (MD) simulations were invented as a tool to study thermal properties of condensed matter less than 50 years ago, two general problems have come into focus: fluid properties and phase transitions. Of course, statistical thermodynamics provide a general framework to deal with such questions, but apart from rare (and fairly academic) perfectly soluble models, quantitatively accurate results of the analytic theory of materials were mostly restricted to dilute gases, dilute solutions, perfect crystals, and so on. Even the simplest phase transition descriptions (such as van der Waal's gas-liquid transition theory) are rather poor. They're unreliable in all quantitative aspects and misleading in qualitative aspects, especially near critical points in the phase diagram.

Fortunately, we've reached a better state of affairs for simple systems for which reliable, effective potentials based on quantum chemistry are available. We can study their detailed structure and phase transitions with classical Monte Carlo methods (the computer samples the system's microstates with a probability proportional to the Boltzmann factor using random numbers) or the MD method (the computer numerically solves the particle system's Newton motion equations).[1] In recent studies, Nigel Wilding accurately described the liquid-gas transition,[2] Kurt Binder clarified critical phenomena in various systems,[1] and Peter Nielaba made accessible low-temperature solid-phase properties (where the path-integral Monte Carlo method can include quantum mechanical effects[3]).

The situation is less favorable for complex materials such as polymeric materials, surfactants, and so on. While we can perform atomistically realistic simulations in special cases (molten polyethylene at high temperatures[4] or polyethylene crystals in the orthorhombic phase[5]), these calculations are cumbersome due to potential complexity, and phase transition studies are out of reach. This is even more true for polymer blends, where characteristic length scales occur far larger than the polymer coil's size (which is already of the order of 100 Å, and characteristic time scales range from 10^{-13} sec (bond-angle vibrations) to 10^{-3} seconds (phase separation kinetics).

Nevertheless, useful research on phase transitions in macromolecular systems is possible—we can invent models where complicated local geometric and chemical structure details have been incorporated with a few effective parameters. The idea is to use a coarse grain along a polymer chain's backbone—several chemical bonds combine into one effective bond, and the effective monomers connected by these bonds are the basic degrees of freedom "moved" over the simulation's course.[6]

With this approach, it becomes possible to ask questions such as this: how does a partially miscible polymer-blend phase diagram change due to confinement in a thin-film geometry?[7] Such a question is relevant because thin polymeric layers have many applications for various purposes (such as protective coatings against corrosion). This thin-film geometry has two effects. The first is a predominantly geometric one: the

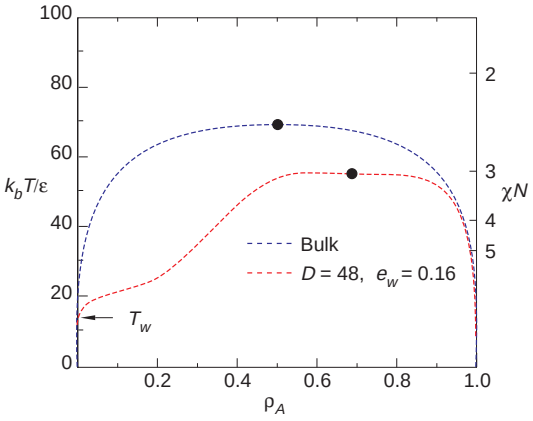


Figure 1. Phase diagram of a symmetrical binary (*A*, *B*) polymer mixture (chain lengths $N_A = N_B = N = 32$ effective monomers) in a thin film.

linear dimension perpendicular to the film is much smaller than the parallel one, hence it limits large-scale growth of inhomogeneity. The other effect is that at a binary mixture's surface, one species is typically energetically preferred over the other: at the surface of a semi-infinite system, even a wetting transition can occur (a macroscopically thick enrichment layer forms). Figure 1 shows how remnants of this transition strongly affect a thin, binary, polymer film's phase diagram. Notice how the coexistence curve exhibits a "bulge" at temperatures just above the wetting transition temperature on the B-rich side of the phase diagram. The region in the T, $?_A$ plane where the mixture stays compatible (no macroscopic phase separation) is strongly enhanced.

In the figure, film thickness D equals 48 lattice spacings for the case where species A is attracted by the walls with an energy parameter $\varepsilon_w = 0.16$. The temperature T (at the ordinate axis) is measured in units of an effective repulsive energy ε between unlike monomers (this scale can be translated into the Flory-Huggins parameter χ, familiar in polymer science). The abscissa is species A's volume fraction. The arrow denotes the wetting transition's location. The coexistence curves between the A-rich phase (in the right half of the figure) and the B-rich phase (in the left side) end in critical points denoted by a dot. Above the coexistence curve, the system is homogeneous on large scales, and a state point below the coexistence curve corresponds to a two-phase mixed state (in the thin film, this means a lateral phase separation).[7]

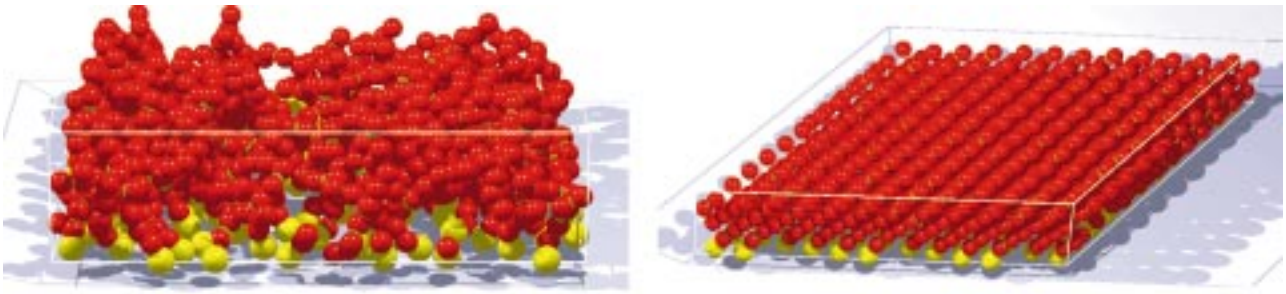
Analytic theories cannot study such phenomena reliably. Well-known theories for polymer blends are the Flory-Huggins and self-consistent field theories. They both predict simple parabolic shapes of the coexistence curve near

$$Tc\{\Delta\rho = \rho_A^{A-rich} - \rho_A^{B-rich} \alpha(1 - T / T_c^{1/2}\}$$

while the actual shape is much flatter {bulk: $\Delta\rho \propto (1-T/T_c)^{0.325}$, thin film: $\Delta\rho \propto (1-T/T_c)^{1/8}$} and T_c is depressed. The analytic theories locate it for $k_BT_c/\varepsilon \approx 84$, for example, $\chi_cN = 2$, in the bulk, while actually it occurs for $k_BT_c/\varepsilon \approx 69.3$. For the thin film, the analytic theory overestimates T_c by 38%.[7]

Figure 1 thus gives an idea how such simulations test corresponding analytical theories and insight into why (and under which conditions) they work or fail. Note also that the lattice unit used in the simulation physically corresponds to about 2Å therefore the film thickness in Figure 1 is about 10 nm, and the lateral linear dimensions ($L = 256$) are about 50 nm. Thus one can work with lattices $L \times L \times D$ of about 3 mio lattice sites, with nearly 10,000 polymer chains in the simulation volume.[7]

We use similar techniques in simulations devoted to understanding the phase behavior of Langmuir monolayers, which are formed from surfactant molecules (such as fatty acids, for instance) at the air-water interface. The water molecules are not included explicitly—rather the hydrophilic head group is fixed in the plane $z = 0$.[8] Because we wish to describe the melting of this layer (the head groups may form either a fluid layer or a triangular 2D crystal), a lattice model similar to the polymer blend previously discussed would be inappropriate. Rather, we would use a bead-spring model in the continuum for the surfactant's hydrophobic alkane



(a) (b)

Figure 2. Configuration snapshots of a Langmuir monolayer model, using a model of grafted stiff chains with Lennard-Jones forces among the beads: (a) the disordered expanded phase (LE), and (b) the condensed modulated phase LC-mod.[8]

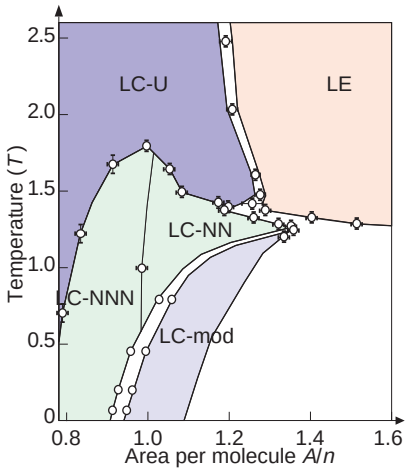


Figure 3. Phase diagram of Figure 2's model. LE denotes a disordered expanded phase, LC-U a condensed phase with untilted chains, LC-NN and LC-NNN condensed phases with collective tilt toward nearest neighbors and next nearest neighbors, respectively, and LC-mod denotes a phase that has a superstructure and an intermediate tilt direction.[8]

chains, with a bond-angle potential for the effective bonds.[8] Figure 2 proves that the phases of interest can be modeled. Because the chains in the regular stretched configuration still have cylindrical symmetry, unlike the real alkane chains in their all-trans zig-zag configuration, the model is invalid for a description of the various crystalline Langmuir monolayer phases. But the various liquid (and liquid crystalline) phases can be modeled, as in Figure 3, and we can learn how changes in the model's control parameters such as head-group size relative to effective monomer size and so on affect possible phase transitions.

From these examples, it's apparent that the goal of such simulations is not to predict numbers but to provide understanding. But such approaches are clearly useful for experiments. For example, it was first discovered in a simulation[9] and later confirmed by an experiment that a polymer brush (where flexible chains are end-grafted at a surface) in a bad solvent might undergo a microphase separation from a homogeneous to a laterally inhomogeneous state. This situation is undesirable for applications, and we need to understand the conditions to avoid it.

There is much recent interest in self-organization of structures formed by complex molecules in a hierarchical way. Simulation studies of such phenomena are urgently needed to clarify the role of control parameters for such ordering phenomena. Even more complex structures and transitions between them occur in biological systems and related contexts (such as biomineralization). Vast and largely unexplored fields still exist for which simulation studies as described here still have to be developed, and rapid progress in the near future can be anticipated.

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EDUCATIONAL SOFTWARE AND THE SISYPHUS EFFECT

Wolfgang Christian

IN 1991, DAVIDSON COLLEGE HOSTED THE SECOND NSF-SPONSORED CONFERENCE ON COMPUTATIONAL UNDERGRADUATE PHYSICS. OVER 125 PHYSICISTS FROM THE UNITED STATES AND FOUR FOREIGN COUNTRIES ATTENDED the four-day event. This conference offered the unique feature of giving each participant a computer account and asked that each bring and share software and curriculum material. Within hours of open registration, 350 megabytes of programs (but almost no images or text) appeared on the server. Almost every participant contributed a small homegrown DOS or Apple II program.

During the conference, it was common to see participants sitting at a computer with stacks of floppy disks, ready to download and take home files for the eventual computer-enabled educational revolution that we all anticipated. It didn't happen—at least not in the form the conference participants envisioned. The mainstream teaching community adopted little of the conference software, and almost none of it is still in use today.

In contrast, printed material from the much earlier, post-Sputnik curricular reform movement (the Berkeley Physics series, for instance) is still available and useful to physics educators, although the pedagogy upon which it was based has gone out of fashion. Will this scenario repeat, dooming us like the Greek hero Sisyphus to forever push computational physics up the hill of curriculum reform? Can we expect widespread adoption of computation in the current curricular reform initiative? And if so, what strategies should we adopt to insure the acceptance and widespread use of the computationally rich curricula being developed today?

Authoring

The rapid pace of hardware and operating-system development made it difficult for text and software authors to produce computationally rich curricular material that was not obsolete shortly after publication. The half-life of a typical computer desktop was shorter than the textbook publication cycle, and this all too often led to minimal documentation, poorly tested nonstandard user interfaces, and idiosyncratic behavior.

Computational physicists accustomed to programming in Fortran had little interest in page-layout and user-interface design. The tools scientists used in daily office work, such as correspondence, class management, and professional publication, interoperated poorly with programming tools and educational software. Publishers were therefore reluctant to integrate computer use into primary educational texts, and the mechanism to effectively create and distribute media-rich documents from the desktop simply did not exist.

Not surprisingly, many thoughtful teachers were unwilling to invest time and energy to overcome these obstacles. Because little research had been done on the effectiveness of computer-based instruction, this wait-and-see approach might have been wise. But the case can now be made that this throw-away cycle for educational software need not repeat itself and that key technologies now exist that let programmers author and distribute curricular material that will withstand the test of time.

The most promising technologies are based on virtual machines, metalanguages, and open Internet standards. These technologies are platform-independent. The marriage of word processing and desktop publishing with Internet technologies is already taking place. The current generation of desktop applications is Internet-aware (that is, they can embed HTML anchors and export static Internet content), and the next generation will be Internet-centric. Authors already download documents from servers, edit them in a Wysiwyg environment, and upload them back to the server. Extensible markup language and cascading style sheets will soon provide rich formatting and enable context-sensitive searching and indexing of these electronic documents. Manufacturing, inventory control, and advertising have, in effect, provided the education community with a rich and flexible set of standards to enable electronic curriculum distribution.

Interactive engagement

Although the Internet lowers the barriers to authoring and distributing educational software, its long-term ability to deliver active content might be more significant. Much of the current curricular reform effort in physics is based on the idea of *interactive engagement*. In a widely respected article, Richard Hake compared the cognitive

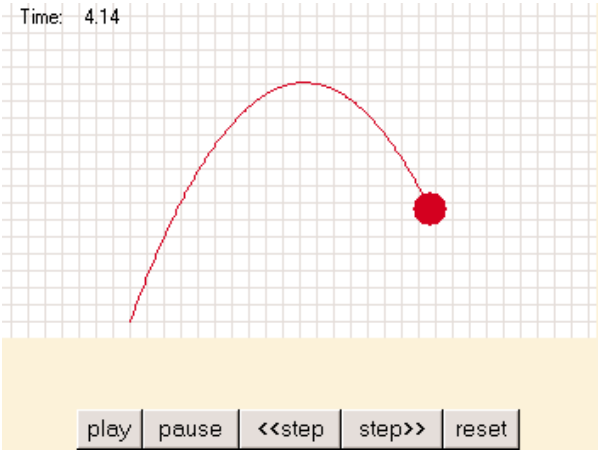

Figure 1: The Animator Physlet scripted to show a projectile problem.

gains of IE classes to traditional lecture-based classes.[1] Hake defines interactive engagement methods as

> …those designed at least in part to promote conceptual understanding through interactive engagement of students in heads-on (always) and hands-on (usually) activities, which yield immediate feedback through discussion with peers and/or instructors.[1]

This study showed a significant improvement in understanding IE methods using a standard instructional diagnostic—the Force Concept Inventory test.[2] To become an effective educational tool, computers must foster the IE approach using commercial mass-market technology. The Java programming language coupled with a scripting language such as JavaScript is likely to play a leading role in developing this type of curricular material.

We have been using Java technology at Davidson College to develop a set of small scriptable applets—we call them Physlets—capable of displaying physics content.[3] (Visit *http://webphysics.davidson.edu* to find Physlets and Physlet problems.) Because Physlets are embedded into text documents and are scriptable, we can easily use them for concept tests, homework, prelabs, and in-class demonstrations. In designing interactive material, it is useful to distinguish between media-enhanced problems—where multimedia presents what is described in the text—and media-focused problems—where the student uses the multimedia elements to solve the problem.

Multimedia-focused problems differ fundamentally from traditional physics problems, and Physlets are ideally suited for these types of problems. For example, the traditional projectile problem states the initial velocity and launch angle and asks the student to find the speed at some point in the trajectory. This problem can be media-enhanced by embedding an animation in the text, but this adds little to the problem's value.

Alternatively, this same problem can be a media-focused Physlet problem as Figure 1 shows. In this case, the text does not give the numbers. Instead, students must find the minimum speed along the trajectory and observe the motion, apply appropriate physics concepts, and measure the parameters they deem important within the Physlet. (A mouse-down movement enables them to read coordinates.) Only then can they solve the problem. Such an approach differs remarkably from typical novice strategies, where students attempt to mathematically analyze a problem before qualitatively describing it (an approach teachers often call "plug-and-chug").[4] Requiring students to consider problems qualitatively has had a positive influence on students' problem-solving skills and conceptual understanding.[5,6]

JiTT

Although technology provides pedagogically useful media-rich content and interaction, it lacks the human dimension important for effective teaching. *Computer-assisted instruction* has, after all, already been tried on very elaborate proprietary systems. It is unlikely that porting it to the Internet will cause significant improvements. To be truly effective, the computer's communication capabilities must create a feedback loop between the instructor and student.

A new and particularly promising approach known as *Just-in-Time Teaching* (JiTT) has been pioneered at Indiana University and the United States Air Force Academy and further developed at Davidson College.[7] It employs a fusion of high-tech and low-tech elements. On the high-tech side, it uses the World Wide Web to deliver multimedia curricular materials and manage electronic faculty and student communication. On the low-tech side, the approach requires a classroom environment that emphasizes personal teacher-student interactions. It combines these disparate elements in several ways, and the interplay produces an educational setting that students find engaging and instructive. The underlying method creates a synergy between the Web and the classroom to increase interaction and allow rapid response to students' problems.

The JiTT paradigm is most closely associated with the interactive lecture session. Short Web-based assignments—designed to encourage students to assemble any prior knowledge they have about the upcoming topic—are due just hours before class. The instructor then builds the class session around the students' answers, taking this opportunity to discuss the their work.

The typical student needs to preview the material in the textbook to complete the assignment. The instructor collects the students' electronic sub-

missions, reads them, and presents excerpts from them during class, weaving them into the lesson as appropriate. Thus, the students take part in a guided discussion that begins with their own preliminary understanding of the material. Instructors do not simply go over the student responses in an isolated section before or during a lecture, rather, they frame their lecture and classroom activities by analyzing various student responses.

Although it would be foolish to predict the future direction of computer science and the computer industry, physics education research informs us that technological advances do not necessarily lead to improved learning. For example, streaming video is currently a hot technology, and both traditional broadcasters and software companies compete to establish themselves in this market. But PER has shown that merely watching video has little effect on student learning, and it is unlikely that streaming large video files will change this result.[8]

Small cognitive effects have occurred using video clips—if the clip is accompanied with in-class discussion or used for data-taking and data analysis. Similarly, database technology has become ubiquitous in our society. It can store consumer-shopping profiles for corporate marketing departments and manage Christmas card mailing lists at home. But we have gained little by using database techniques to track student learning and tailor curricula to individual learners.

Other high-end technologies, such as virtual reality, 3D modeling, and voice recognition, will almost certainly come online in the coming decade. However, their most enduring effect on education might be to drive the price-to-performance ratio of consumer—and hence educational—hardware even lower. These technologies are unlikely to have a significant impact on undergraduate education without a corresponding curricular development effort. Current commercial technologies might, in fact, already be good enough to implement the most effective teaching strategies. Unlike previously written educational software, software written using current Internet standards should be accessible for years to come. But for computation to have a long-lasting impact on science education, we will need to based it more on successful pedagogy than on the latest compilers, hardware, or algorithms. CiSE

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COMPUTERS AND THE PARTICLE THEORIST

Michael Creutz

IT GOES WITHOUT SAYING THAT COMPUTERS ARE NOW ESSENTIAL TO ANY SCIENTIST'S WAY OF LIFE, INCLUDING THE PARTICLE THEORIST. WALK DOWN THE HALLS AND COUNT THE PERCENTAGE OF YOUR COLLEAGUES currently sitting in front of a terminal. One of the most exciting features of these developments is the entwining of interdisciplinary activities with the growth of computing in science.

As science has grown more complex, a natural specialization has occurred. Many closely related ideas are rediscovered independently with divergent jargon. The computing revolution has slowed and occasionally even reversed this trend. Numerical difficulties with hadronic physics at large baryon density are mathematically equivalent to doping issues in many-electron models for the perovskite superconductors. Particle physicists are striving to adapt *cluster* algorithms from statistical mechanics to their own simulations. The numerical lattice-gauge simulations arose directly from methods developed in the condensed-matter community. Going beyond pure science, recent studies of interacting *agents* have created a new field sometimes loosely referred to as *econophysics*. New algorithms for track detection in high-energy detectors closely relate to scheduling problems in commerce.

In the early 1980s, I wrote an essay[1] on the role of computers in high-energy physics. When I look back at that article, many of the same issues remain valid today—a rapidly growing need for cycles and a continual technology push. Experimentalists are probably still the major computer users, but they are less vocal than the lattice-gauge theorists with their large machines. Beyond analyzing huge numbers of events, it is amazing to what extent we can accept that a new experimental result relies on sophisticated statistical analysis to extract a few unusual events from huge backgrounds. The discovery of the "top" quark and the observation of the extremely rare decay of the charged kaon to a pion and a neutrino-antineutrino pair are two particularly striking examples. Meanwhile, computation-intensive phenomenology has grown into a highly respected part of the theoretical community required to understand complex experimental data.

The last two decades have seen a continuing evolution in the way theoretical particle physicists view and use computers. The empirical demonstration of quark confinement in non-Abelian gauge theories showed that computer simulation could provide deep insights into nonperturbative effects in interacting quantum field theories. Now that confinement is accepted as a theory property, we debate in a nuclear-physics style about possible mechanisms. Lattice-gauge theory has evolved into a mature subject, capable of concrete predictions on such issues as glueball masses and disentangling weak mixing angles. Many of the old problems remain, with theorists still arguing about how to handle fundamental issues such as fermion doubling or lattice topology. Fermion simulation algorithms have become fairly standard, though old unresolved issues, such as including a chemical potential or odd numbers of species, remain.

As computers have gained in power and become basic tools, the concept of CPU time as a valuable resource is finally fading. My personal $1,000 laptop is considerably more powerful and more friendly than the $10,000,000 CDC 7600 I worked with 15 years ago. Only the most major computational science projects still worry about machine hours as money. With the explosion of networking, computational strength is no longer measured primarily in terms of a single machine's horsepower.

Many computer uses have crept insidiously into our lives. The essentially complete replacement of conventional mail and the telephone in the scientific community is the prime example. When was the last time you got a phone call that wasn't a wrong number or someone begging? With the growth of computer networking, the traveling physicist maintains e-mail contact throughout his voyages. Indeed, conference organizers that ignore these addictions are quickly chastised.

The success of the computer preprint archives has been phenomenal. It is easier for me to check my own publication information on the Web than to find the papers on my own office shelves. The postcard reprint requests so common a few years ago have all but disappeared. The journals themselves are being forced to adapt to this revolution, although they are still in a state of flux with rough edges. Now a paper can proceed from first draft to journal printing with the only

ink appearing on the copyright transfer form. Soon even journal print versions might disappear when displays acquire magazine portability.

Another consequence of the networking revolution is that one rarely interacts with a single computer at a time. Our files stay on a central server, and we run intensive computations on another machine, while a third piece of hardware occupies our desk and provides access. In my ongoing exploits on the RIKEN/BNL QCDSP Supercomputer, I have nearly simultaneously edited source code on my local workstation, run simple debug tests on a shared ultra-sparc, compiled for QCDSP on a machine at Columbia University, and linked to it through its host workstation and then on the supercomputer itself. This represents five distinct machines, all accessed transparently and concurrently through scripts on my local workstation. A computer is ceasing to be a single entity—it's now a small piece of the system.

The Web, of course, is the most visible, unanticipated effect of computers on science—indeed on society as a whole—but enough has been said about that elsewhere. We should, of course, remember with pride that it was high-energy physicists that invented this concept. It is merely conservative to anticipate further wildly unexpected applications.

The spreading of networking has had the side effect of forcing standards to reduce the Tower of Babel in computing. Web browsing on PCs, Macs, and Unix boxes is essentially equivalent. E-mail messages containing attachments in unusual formats are a bane rapidly being banished. Soon all our communication will be based on some variation on extensible markup language. The Web is also beginning to replace other ways of communicating with colleagues. You can drop notes into a public directory and tell colleagues where to find them. This raises security issues that appropriate encryption can easily solve.

The issue of privacy is one that most physicists have ignored.

In this vein, the issue of privacy is one that most physicists have ignored. While the major journals all now ask to receive referee reports by e-mail, they scoff at the suggestion that they should provide public keys for encryption or verification of potentially sensitive or modifiable material. I digitally sign reports, but I doubt that these are ever checked. Either this will change as the vulnerabilities of electronic transmission become better appreciated, or more likely the issue will disappear as encryption becomes invisibly built into the infrastructure.

Despite the empowerment, rapid communication has some negative effects. Most noticeable is the feeding of impatience. People expect immediate responses to their e-mail messages, knowing that the excuse of a slow postal service is no longer valid. The ease of sending messages impulsively and the obscurity of electronic irony often cause unnecessary and unexpected misunderstandings. Meanwhile, the universality of networking has brought a trend toward centralized computing back. This frightens me a bit, having seen the freedom of being independent of large infrastructures, and it is a bit surprising given the astounding growth of PC power. This fear hit close to home recently with a multiday failure of our laboratory's entire networking infrastructure. But I suppose as things evolve, so too will redundancy. Each individual computer will be more like a single cell in a large organism, continuing to function even if a few pieces are scraped off. A harddisk failure will be nothing more than a minor scratch.

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